Reproducible research with R

19th June 2013

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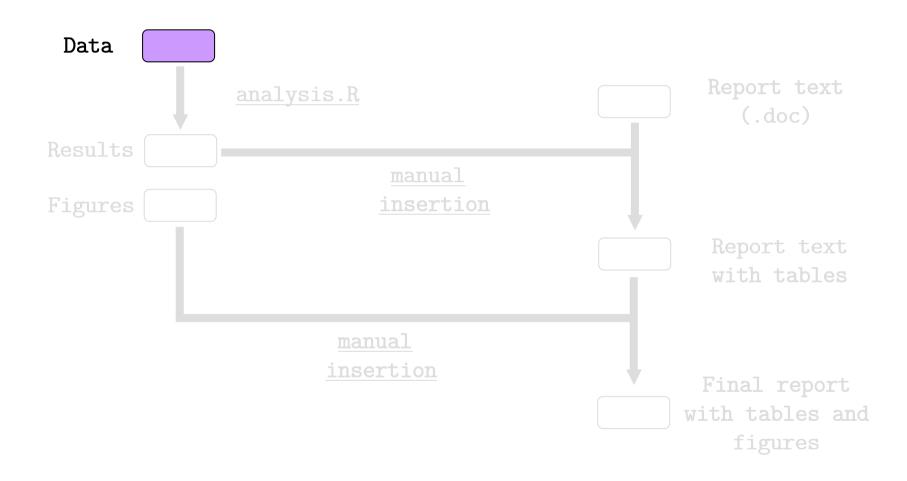
Report generation Tools

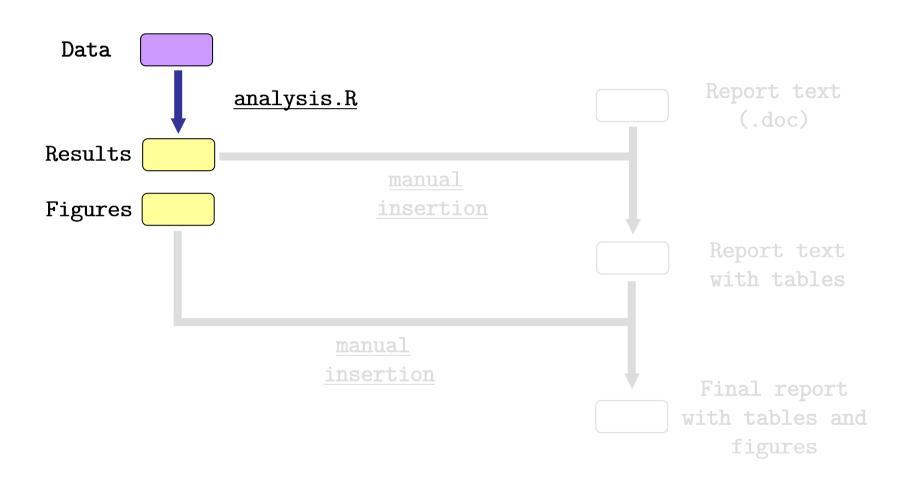
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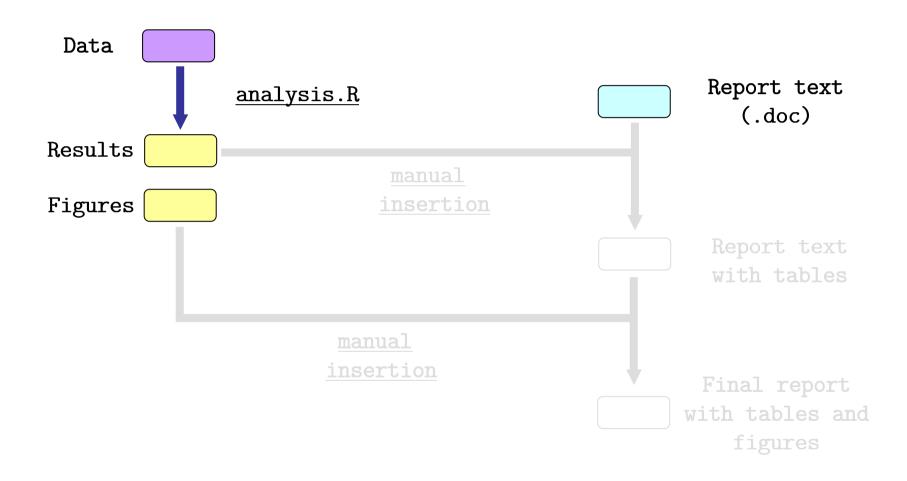
 Sweave and LaTeX – PDF output Latex

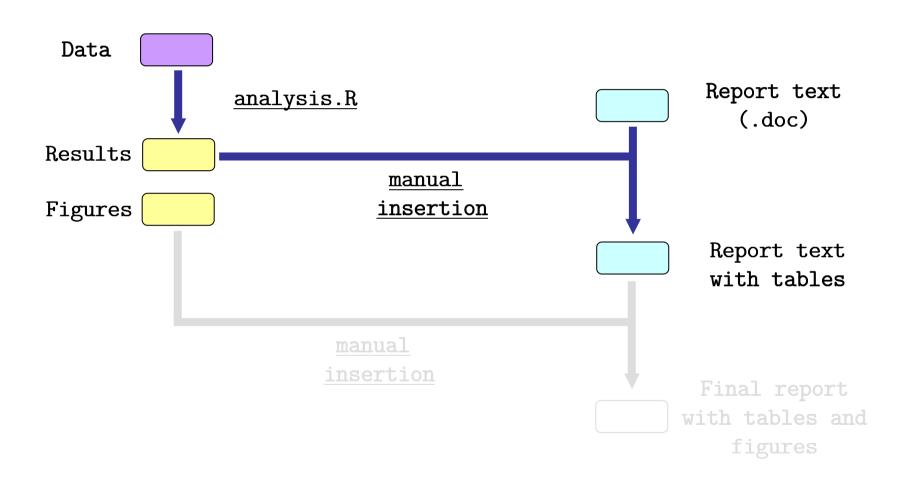
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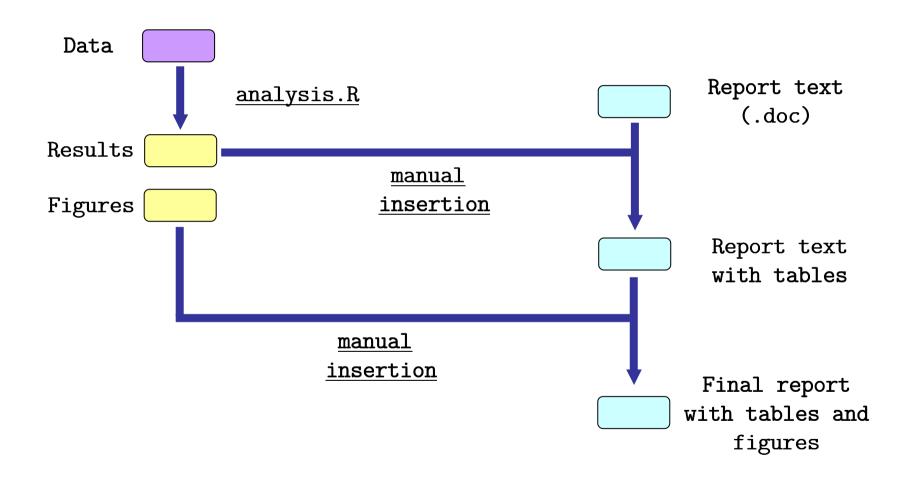
Part II Report generation

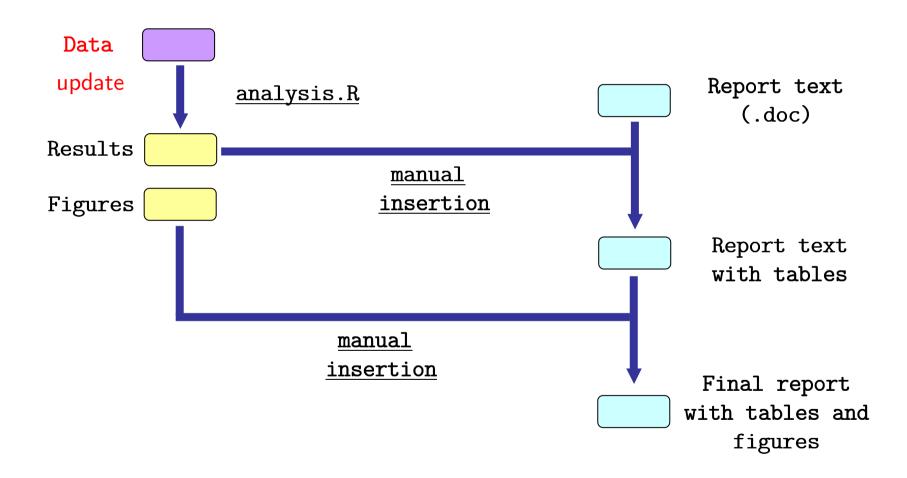


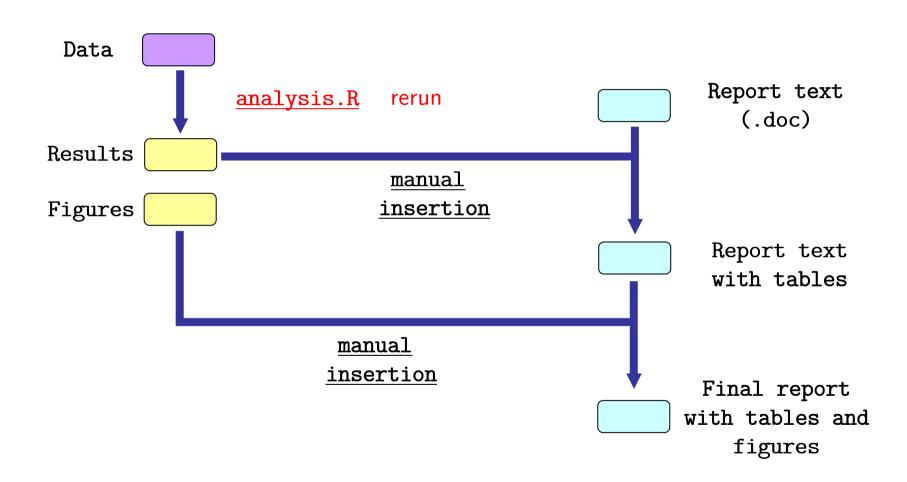


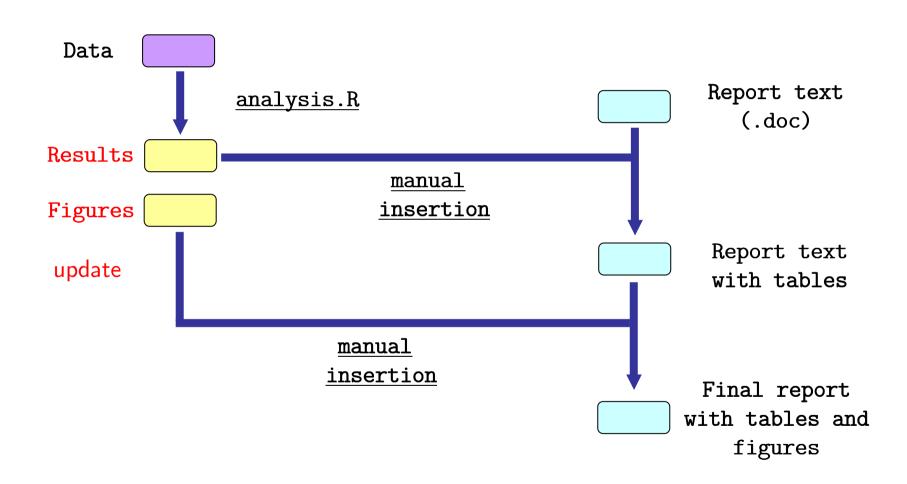


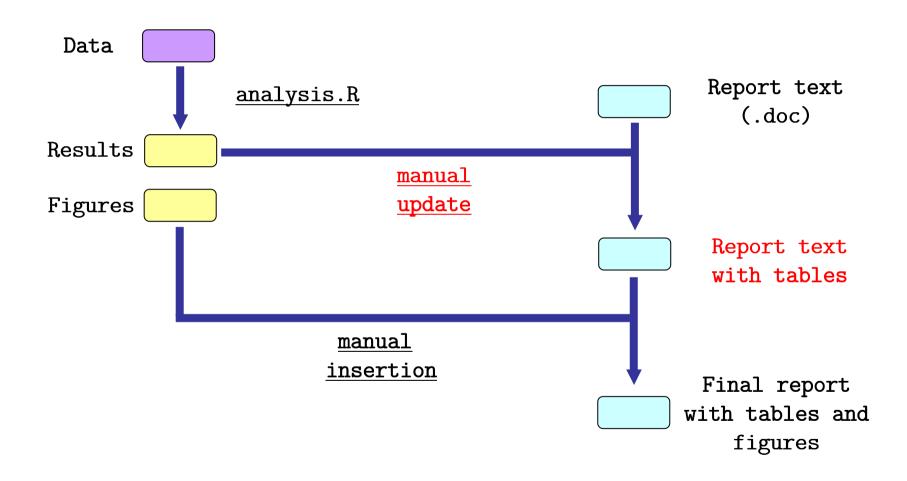


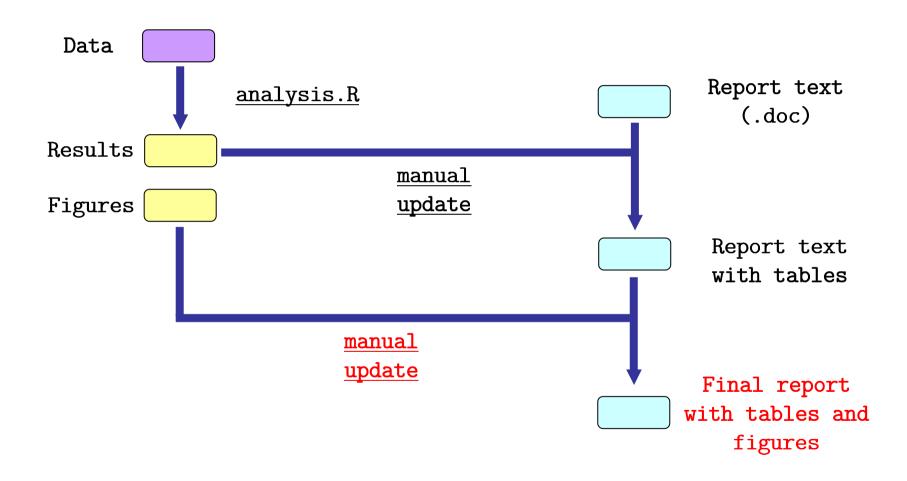








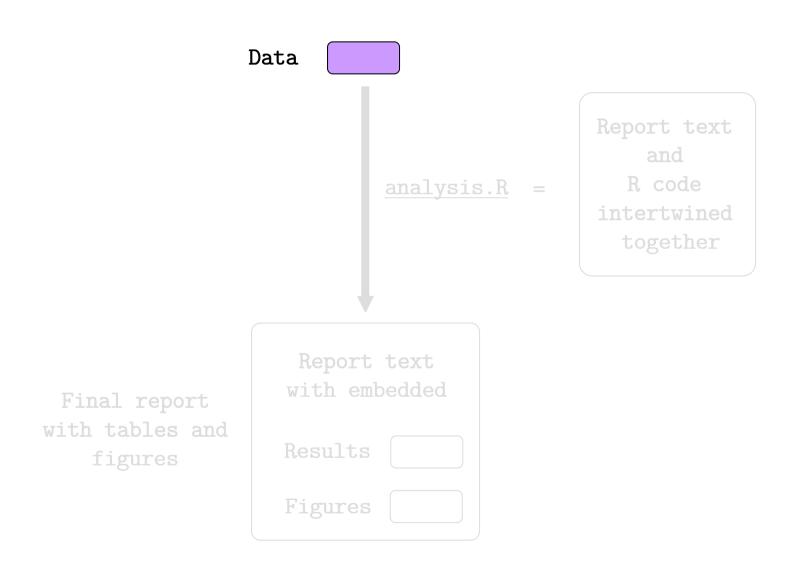


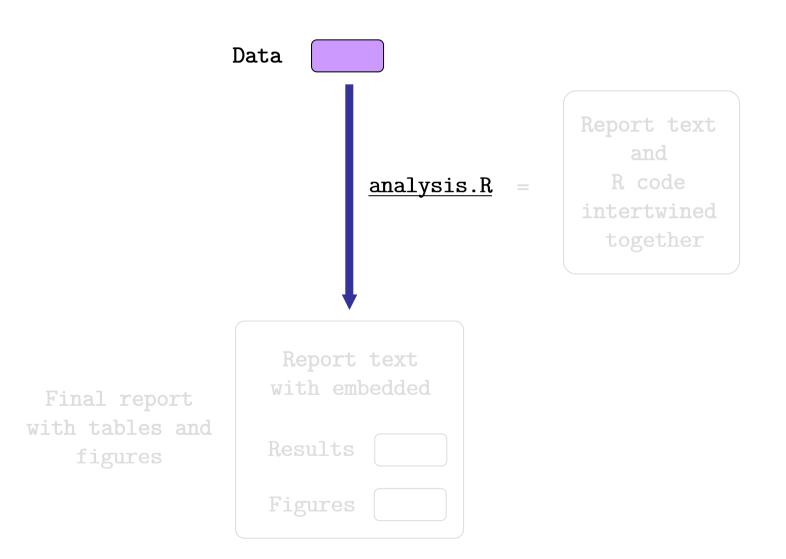


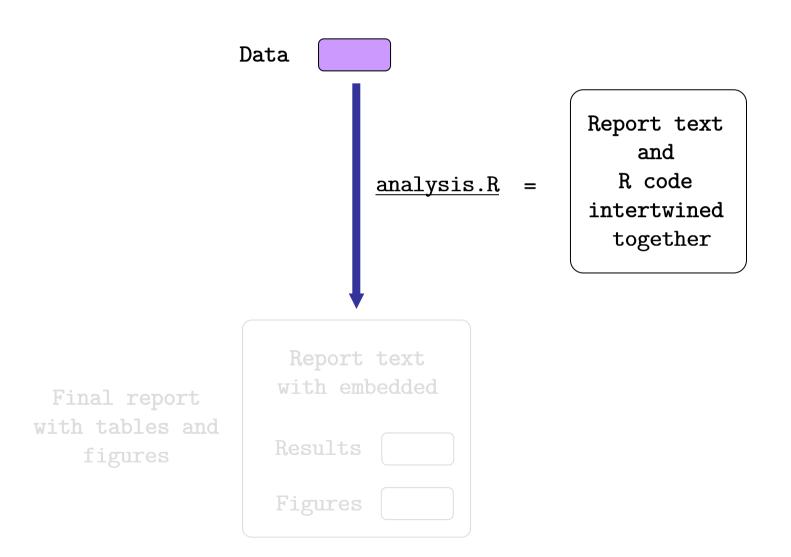
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- It is also error prone.
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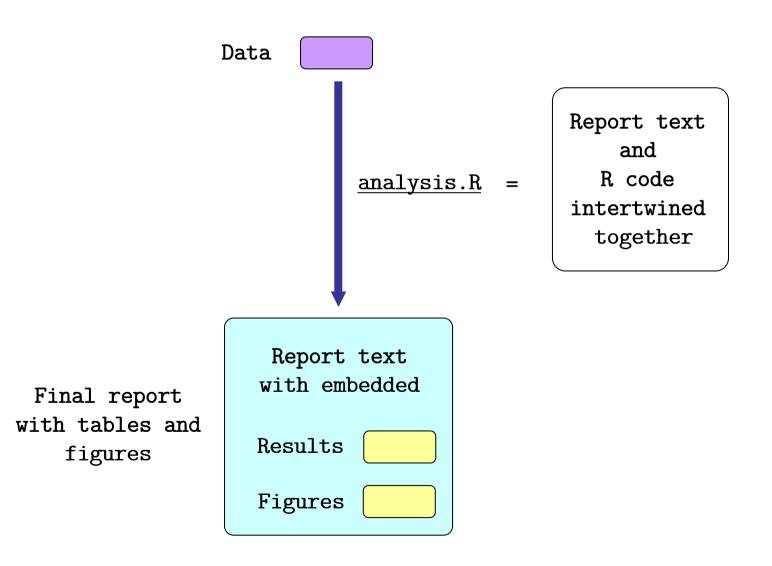
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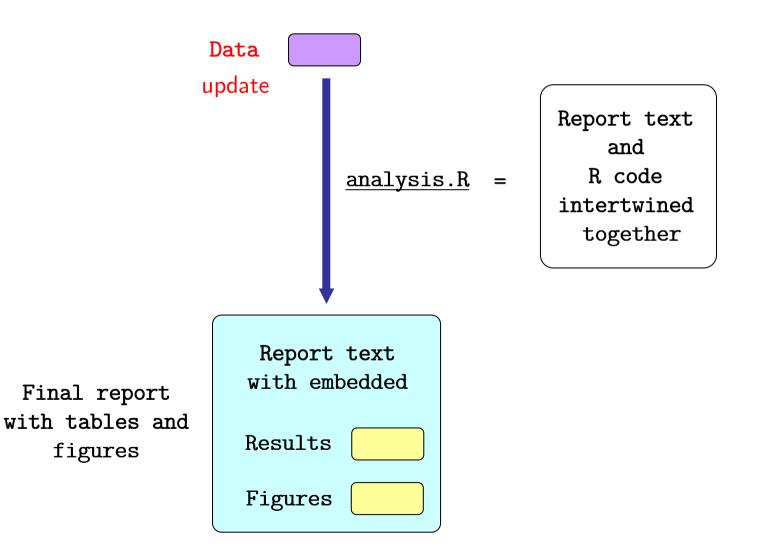
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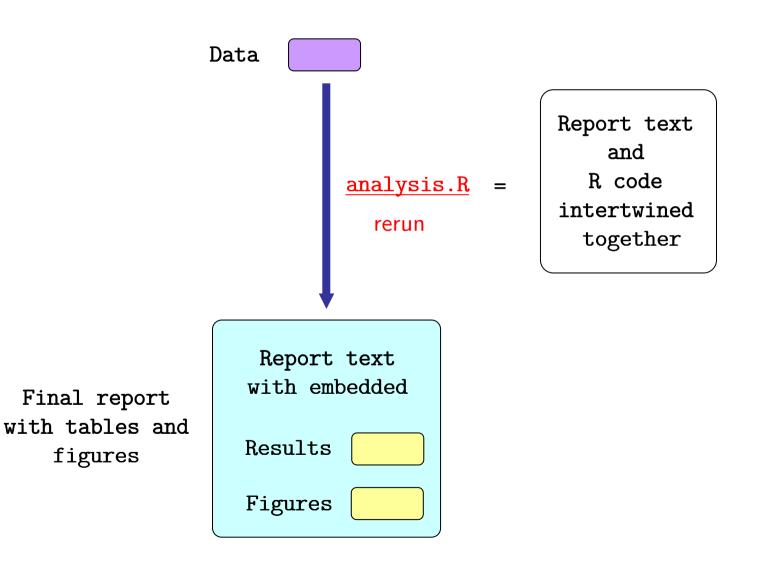


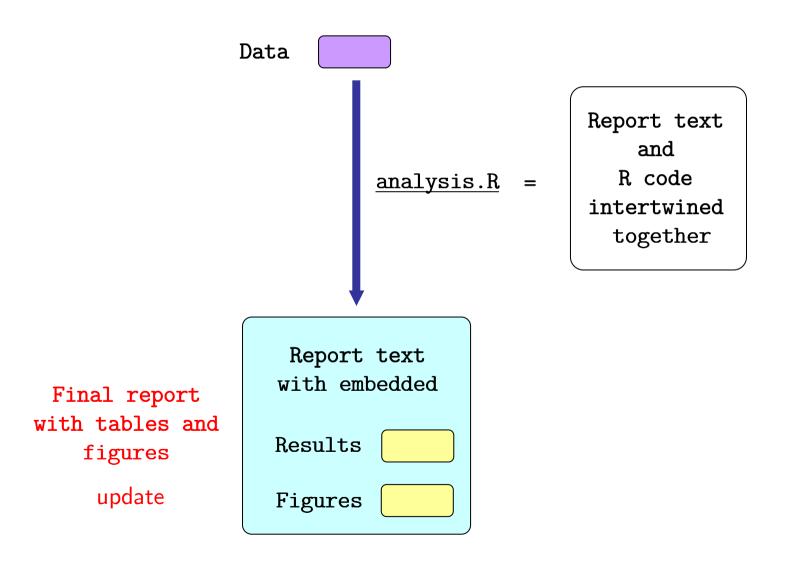












- Data analysis, comments and interpretation are mixed together in the R script, as it is in reality.
- The final report is produced automatically and can be updated in a single step.
- The report generation script can be version controlled!

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Scripts with R code and regular text mixed

```
Temperature evolution
We could study the temperature evolution of Turun Yliopisto
duck pond using publicly available oceanographic data.
This is the **first study** showing an increase in the duck pond
summer temperature over the last 20 years.
```{r fig.width=4, fig.height=4}
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plot(pond$year, pond$temperature)
```

Scripts with R code and regular text mixed

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 plot(pond$year, pond$temperature)
code
```

• The script is interpreted with the regular text being formatted and the R code executed.

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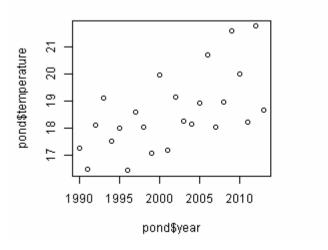
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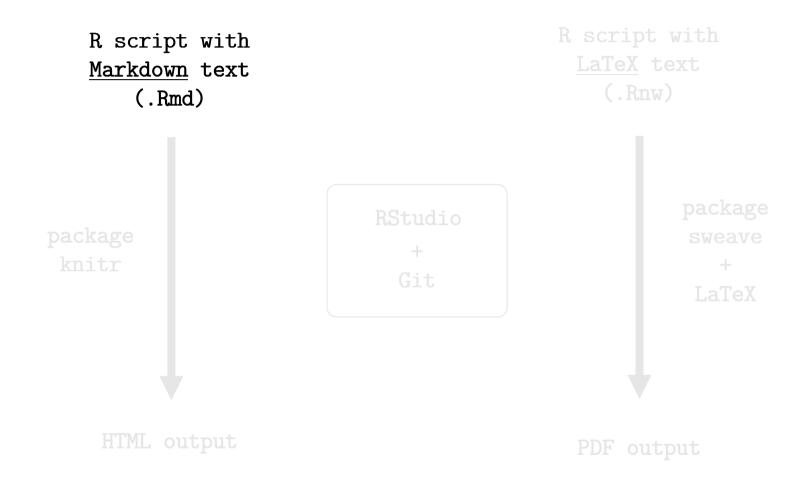
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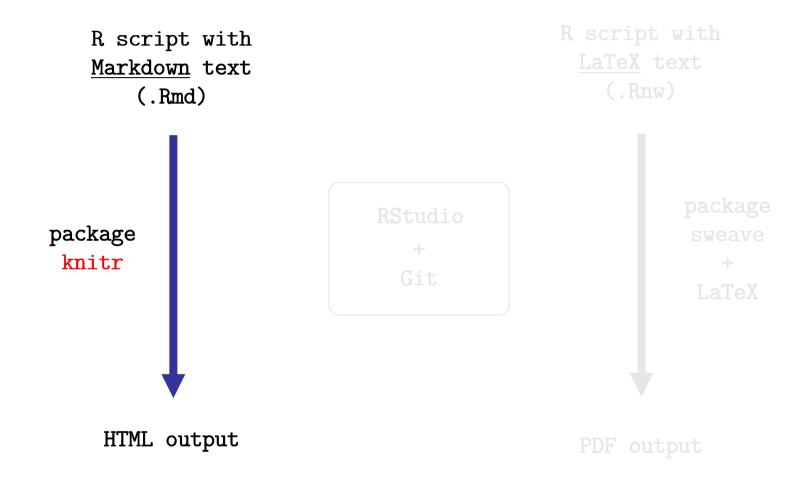
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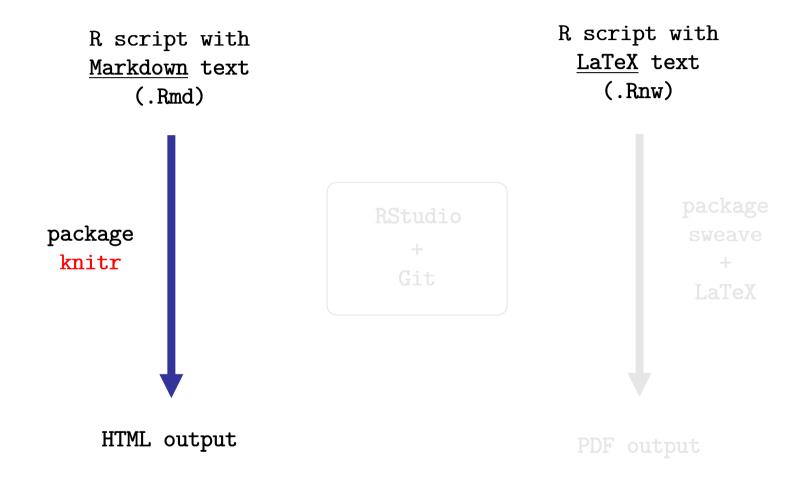
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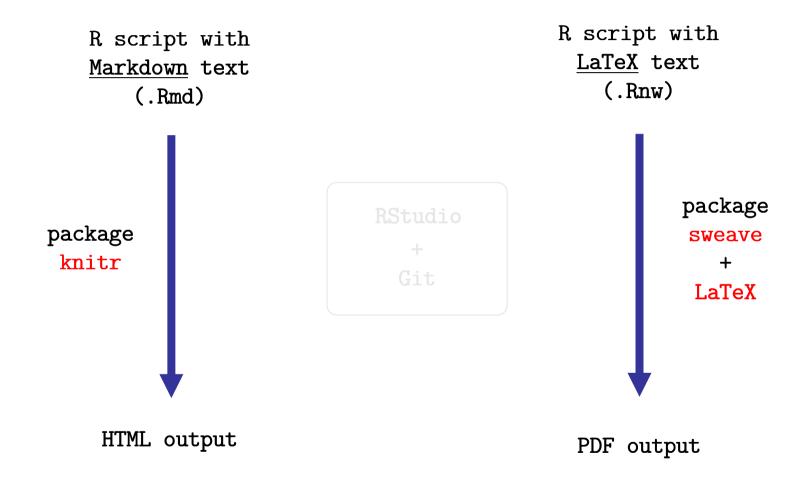
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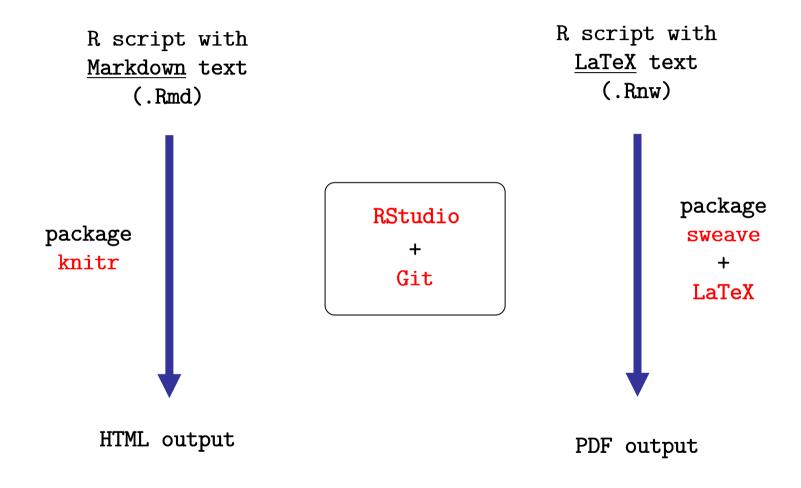












Markdown - HTML output

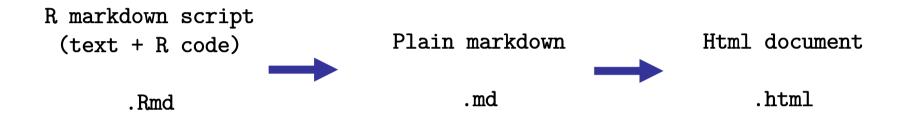
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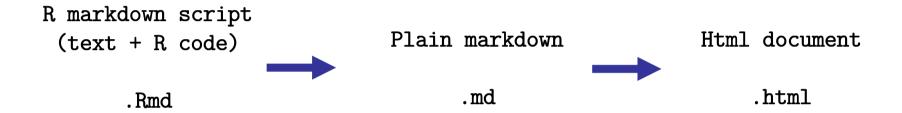
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Markdown - Practical

- We are going to analyse a Moomin related dataset to practice report generation with Markdown and Sweave + LaTeX.
- The exercise folder is report_generation. It contains a data folder with the original data files.
- In case of need, all the code used for the practical is available in the files:

```
moomin_reference.Rmd
moomin_reference.Rnw
moomin_reference_advanced.Rnw
```

- First, let's start a new RStudio session.
- Create a new file by 'File > New > R Markdown'. RStudio puts some code in it by default, erase it and save the empty file as moomin.Rmd in the report_generation/markdown folder ('File > Save as...').
- Note the MD icon on top of the source pane. You can click on it for a markdown quick reference.

Setting up the working directory

- In the 'Files' tab, enter into the report_generation/markdown folder.
- Set it as the default directory by clicking 'More > Set as working directory' on the top of the 'Files' tab.
- This ensures that the relative paths to data files defined in the R code will be correct.

Headers

- Headers can be specified easily by underlining some text.
- Write the following text in the source pane:

Haribo et al. have suggested a correlation between the consumption of liquorice and agressive behaviour, but their previous study on Smurfs remained inconclusive.

Kniting

- You can knit your source file by clicking on 'Knit HTML'.
- This will process the source file and open a preview of the html output.
- The icons at the top of the preview windows enable to open the document in the regular web browser, to see the compilation log or to save the document.

Emphasis

- Text can be formatted to italics or bold with *.
- Modify your script this way and knit it:

Lists

For lists, add this text to your script and knit it:

```
Haribo *et al.* study had 3 major flaws:
```

- they did not describe how they measured agressiveness
- most Smurfs escaped before the end of the experiment
- Smurfs have a low expression level of liquorice receptors, as was later evidenced:
 - 1. in the brain
 - 2. in the liver
 - 3. in the muscle

A bit more text

Add more text to your script and knit it:

Experimental design

We decided to test their hypothesis using a dataset collected on Moomins and other related characters. Our approach includes:

- male and female individuals from different species
- different levels of liquorice consumption among individuals
- paintball activity as a proxy for agressiveness

 Note how the plain-text of the source file is easily readable and already formatted by the markdown syntax itself.

R code chunk

 Time for some code. Add this text to your script and knit it:

• Text delimited by ```{r} and ``` is interpreted as R code and executed when the file is processed. RStudio uses colored background to separate R code from plain-text.

R code chunk

- Each R code block is called a code chunk. Code chunk output is added to the html document.
- Code chunks can be labelled for easy access. Modify your source this way:

```
Individuals used in this study
------
```{r loadMoominData}
Load Moomin data
moomin = read.table("../data/moomin_data", header = T, sep ="\t")
moomin
````
```

R code chunk

• Let's load a bit more data to continue our practice:

```
Results
### Paintball activity
For each individual, the number of used balls during a 180min
paintball game was monitored.
```{r loadPaintballData}
Load paintball data
paintball = read.table("../data/paintball_data", header = T,
 sep = "\t")
head(paintball)
```

### **Graphics**

• We can easily add a plot to the output:

### **Graphics**

• We can also use ggplot:

```
The next plot uses `ggplot2` for fancier graphics.

```{r plotSniffActivity.ggplot2}
library(ggplot2)
ggplot(sniff_activity, aes(x = time.min, y = balls.used)) +
    geom_line()

```
```

 Note the backquotes around ggplot to use the code font in the output.

#### In-line code

 In-line code can be used and evaluated outside of R code chunks :

```
Activity of all individuals
The next plot uses the data for all `r nrow(paintball)`
records in the paintball tables.

```{r plotActivityAll}
ggplot(paintball, aes(x = time.min, y = balls.used, col = user)) +
    geom_line()

```
```

• In-line code must be defined by typing **r** just after the opening backquote.

### R code chunk options

• R code chunk have many options that can be used. Let's make the previous plot a bit wider by modifying our code:

```
Activity of all individuals
The next plot uses the data for all `r nrow(paintball_data)`
records in the paintball tables.

```{r plotActivityAll, fig.width = 8, fig.height = 5}
ggplot(paintball, aes(x = time.min, y = balls.used, col = user)) +
    geom_line()
```
```

#### Hidden code

 We can run R code without displaying it in the final document. This can be useful for intermediate steps of limited interest for the result interpretation.

#### Hidden code

- In the previously added text, note the use of in-line code for the liquorice consumption range. If the data is updated with new individuals, this range will be updated automatically when the report is generated again.
- Using echo=FALSE in the code chunk header makes the code invisible in the html output.
- At this point, note also how you can easily navigate between the code chunks using the menu at the bottom of the source pane.

#### Hidden code

 Hidden code can be used to define functions or run lengthy code without crowding the output:

#### More code

 We are basically interested in the effect of lakritsi on paintball activity. We can start by looking at it graphically:

```
The next plot uses color-coding to depict the average consumption
of lakritsi in kg/day.
```{r plotActivity.col.lakritsi, fig.width = 8, fig.height = 5}
ggplot(all_data, aes(x = time.min, y = balls.used, group = english)) +
   geom_line(aes(col = liquorice.kg.day))
We can also look at the total number of balls used in relation to the
liquorice consumption.
```{r plotTotalBallsLiquorice, fig.width = 8, fig.height = 5}
ggplot(summary_moomin, aes(x = liquorice.kg.day, y = balls.game,
 col = individual)) + geom_point()
. . .
```

### **Error handling**

• Let's calculate some correlation coefficient:

 A parenthesis is missing and knitr stops and gives us a hint about the location of the error.

### **Error handling**

• Let's correct and run it again:

• Knitr runs fine but an error is visible on the html output. When clicking on the log icon, no more information is available since knitr ran correctly. The error was within the R code but was not a knitr related syntax error.

### **Error handling**

 We have to go back inside the corresponding chunk and correct it:

 Now everything runs fine. A warning was produced by cor.test and it is included in the output.

### **Tables**

• Simple tables can also be inserted:

```
Comparison of the studies

Haribo *et al.* | our study
----|----

Smurfs | Moomins
unknown proxy | paintball activity
potential conflict of interest | no conflict of interest
```

- Kniting the source file does not run it within RStudio: the variables are not defined and cannot be accessed from the console.
- Chunks have to be run manually, either one by one or all of them at the same time (menu 'Chunks' on the top of the source pane).
- Typing moomin in the console gives an error. After running all the chuncks within RStudio, moomin returns the Moomin data frame. We can work as usual with RStudio.

## **Summary**

- R markdown is a very simple language with highly readable scripts.
- Its use ensures a tight link between the analysis and the report (the report file and the analysis file are the same).
- The scripts can be version controlled.

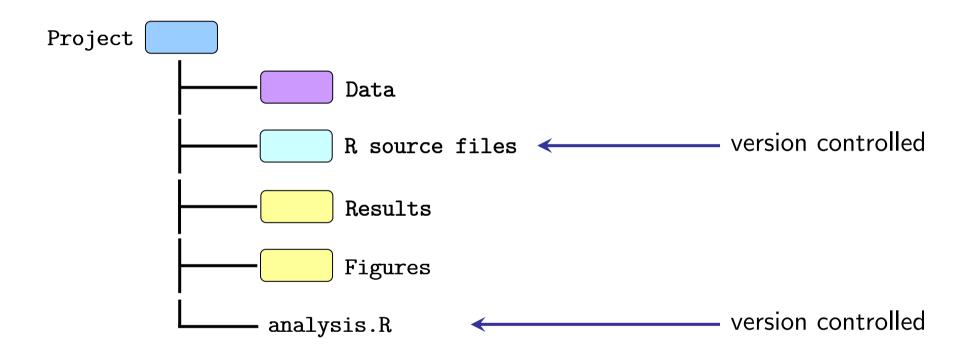
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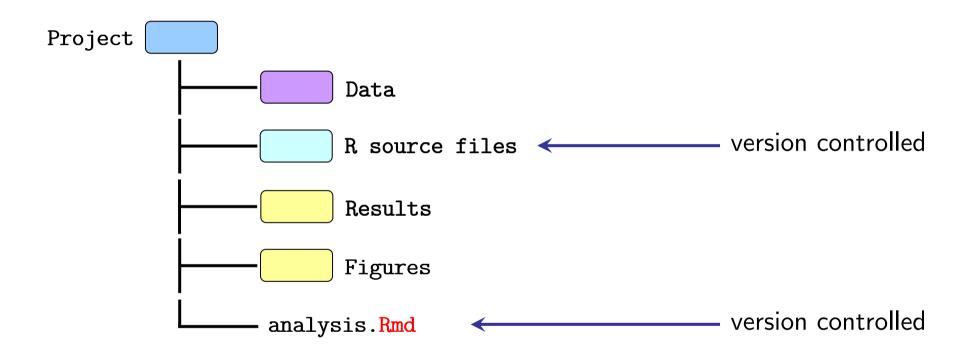
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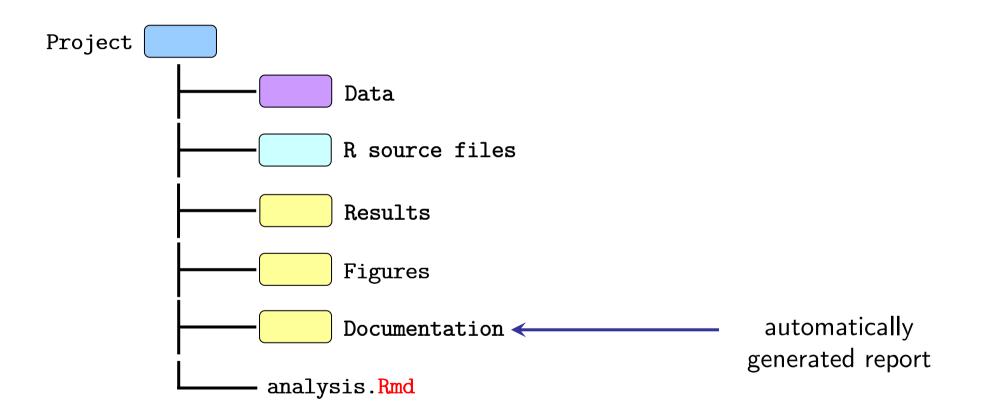
# **Examples of project folder**



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# Sweave + LaTex - PDF output

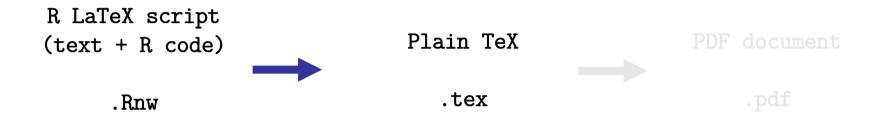
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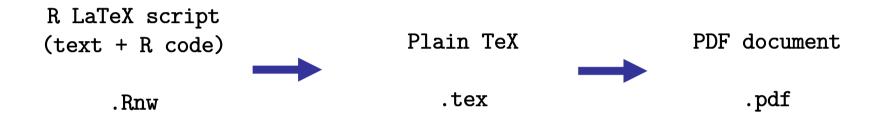
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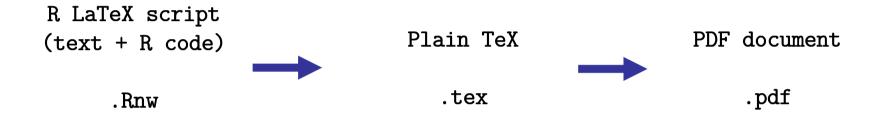
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#### **Disclaimer**

- Sweave is very versatile but is not always very comfortable to use.
- knitr has simplified many aspects of using LaTeX for R report generation.
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# Sweave + LaTeX - Practical

- We are going to analyse the same Moomin related dataset as before to practice report generation with Sweave + LaTeX.
- LaTeX itself must be installed on the computer. A LaTeX distribution is usually quite large (>150 Mb for Windows).
- The LaTeX distribution installation folder should be in the PATH environment variable for Windows OS.

# Modifying the PATH (Windows 7)

- Press the Windows key and the Pause key simultaneously.
- Click 'Advanced parameter settings > Environment variables > Path > Edit...'.
- Add the path corresponding to your LaTeX distribution, separated from the previous path by a semicolon.
- e.g.: C:\Program Files\MiKTeX 2.9\miktex\bin
- Click 'Ok'.

- Let's start by closing all the source files in RStudio and create a new file by clicking 'File > New > R Sweave'.
- Erase the R default code and save the empty file as Moomin.Rnw in the report\_generation/sweave folder.
- Remember that you can use the file moomin\_reference.Rnw if you need it at some point during the practical.

# Setting up the working directory

- In the 'Files' tab, enter into the report\_generation/sweave folder.
- Set it as the default directory by clicking 'More > Set as working directory' on the top of the 'Files' tab.
- This ensures that the relative paths to data files defined in the R code will be correct.

#### Document structure

- Every LaTeX document has a class (e.g. article, book).
- All the printed content must be contained in the document environment, i.e. between the two commands \begin{document} and \end{document}.
- Let's type our very first LaTeX code and save it:

```
\documentclass{article}
\begin{document}

This is a draft about Moomin.

\end{document}
```

#### Document structure

• Click on 'Compile PDF' to start the compilation. The first time, several additional packages might have to be installed by the LaTeX distribution.

A pdf file with only one page is created.

# Title page

• We can create a title page with a few simple commands:

```
\documentclass{article}
\title{Effect of lakritsi on agressiveness: a Moomin perspective}
\author{Matthieu Bruneaux}
\begin{document}

\maketitle
This is a draft about Moomin.
\end{document}
```

## Title page

- We specify some parameters with \title and \author, while the \maketitle command inside the document environment automatically generates a title page.
- Let's save it and compile it.
- The date is automatically added when the title page is built.

### Sections

- A LaTeX document is divided into chapters, sections, subsections and paragraphs.
- For the article class, the chapter subdivision level is not available.
- Let's add the first section:

```
\begin{document}

\maketitle

\section{Context of the study}

This is a draft about Moomin.

\end{document}
```

#### Text

• We replace the draft text by the real one:

```
\begin{document}

\maketitle

\section{Context of the study}

Haribo et al. have suggested a correlation between the consumption of liquorice and agressive behaviour, but their previous study on Smurfs (Schtroumpfus peyoii) remained inconclusive.

\end{document}
```

# Text formatting

Bold font can be obtained with \textbf{}:

```
\begin{document}

\maketitle

\section{Context of the study}

Haribo et al. have suggested a correlation between the consumption of \textbf{liquorice} and \textbf{agressive behaviour}, but their previous study on Smurfs (Schtroumpfus peyoii) remained inconclusive.

\end{document}
```

## **Text formatting**

Italics can be obtained with \textit{}:

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\begin{document}

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\section{Context of the study}

Haribo et al. have suggested a correlation between the consumption of \textbf{liquorice} and \textbf{agressive behaviour}, but their previous study on Smurfs (\textit{Schtroumpfus peyoii}) remained inconclusive.

\end{document}
```

#### Lists

 Lists are more complicated and need a special itemize environment. Each element of the list is defined by the \item command.

```
Haribo et al. study had 3 major flaws:
\begin{itemize}
\item they did not describe how they measured agressiveness
\item most Smurfs escaped before the end of the experiment
\item Smurfs have a low expression level of liquorice receptors, as was later evidenced:
\end{itemize}
```

#### Lists

 Numbered lists can be obtained with the enumerate environment.

```
Haribo et al. study had 3 major flaws:
\begin{itemize}
\item they did not describe how they measured agressiveness
\item most Smurfs escaped before the end of the experiment
\item Smurfs have a low expression level of liquorice receptors, as
was later evidenced:
\begin{enumerate}
\item in the brain
\item in the liver
\item in the muscle
\end{enumerate}
\end{itemize}
```

#### Lists

• Indentation is not necessary but is helpful for the eye:

```
Haribo et al. study had 3 major flaws:
\begin{itemize}
 \item they did not describe how they measured agressiveness
 \item most Smurfs escaped before the end of the experiment
 \item Smurfs have a low expression level of liquorice
 receptors, as
 was later evidenced:
 \begin{enumerate}
 \item in the brain
 \item in the liver
 \item in the muscle
 \end{enumerate}
\end{itemize}
```

#### More text

Let's add the following section:

```
\section{Experimental design}

We decided to test their hypothesis using a dataset collected on
Moomins and other related characters. Our approach includes:

\begin{itemize}
 \item male and female individuals from different species
 \item different levels of liquorice consumption among
 individuals
 \item paintball activity as a proxy for agressiveness
\end{itemize}
```

#### R code chunk

 With Sweave, R code is also contained in chunks delimited by <<>>= and @:

```
\section{Individuals used in this study}

<<>>=
Load Moomin data
moomin = read.table("../data/moomin_data", header = T, sep ="\t")
moomin
@
```

Labels can be added to the chunks:

```
<<label=loadMoominData>>=
Load Moomin data
moomin = read.table("../data/moomin_data", header = T, sep ="\t")
moomin
@
```

#### **Comments**

- LaTeX comments can be added by using % at the beginning of a line, outside code chunks.
- Indentation, empty lines and plain-text underlining using comment lines can help to make the source file more human readable.

```
\section{Experimental design}
%------
We decided to test their hypothesis using a dataset collected on
Moomins and other related characters. Our approach includes:

\begin{itemize}

\item male and female individuals from different species
\item different levels of liquorice consumption among individuals
\item paintball activity as a proxy for agressiveness
\end{itemize}
```

#### More text and code

Let's add the next section and subsection:

## Graph

 One figure can be produced per code chunk. fig and include options have to be set to TRUE for this chunk.

```
\subsection{Example of activity: Sniff (Nipsu)}
This plot shows the amount of balls used by Sniff during the game.

<<label=plotSniffActivity, fig=TRUE, include=TRUE>>=
Extract Sniff activity
sniff_activity = subset(paintball, paintball$user == "Sniff")
plot(sniff_activity$time.min, sniff_activity$balls.used, type =
"1")
@
```

## Graph

 We can also use ggplot, but we need to force the plotting by using a print command.

#### In-line code

In-line code can be evaluated using \Sexpr{}.

#### More in-line code

 A bit more of in-line code which would be updated if the data was to change:

```
\subsection{Effect of lakritsi on paintball activity}

We have an estimation of the average lakritsi consumption per day for each individual. Consumption ranges from \Sexpr{min(moomin$liquorice.kg.day)} to \Sexpr{max(moomin$liquorice.kg.day)} kg per day.
```

#### Hidden code

 Code can be omitted from the output by using echo=FALSE. Useful for lengthy or "boring" code.

```
<<label=mergeTables, echo=FALSE>>=
all_data = merge(moomin, paintball, by.x = "english",
 bv.v = "user")
0
<<label=calculateTotalNumberBalls, echo=FALSE>>=
total.n.balls = vector()
for (individual in moomin$english) {
 total = max(subset(paintball,
 paintball$user == individual)$balls.used)
 total.n.balls = c(total.n.balls, total)
summary_moomin = data.frame(moomin$english,
 moomin$liquorice.kg.day,
 total.n.balls)
names(summary_moomin) = c("individual", "liquorice.kg.day",
 "balls.game")
0
```

#### More code

 Again, let's look at the effect of lakritsi on paintball activity.

#### More code

• And let's see the global trend:

Let's calculate some correlation coefficient:

 A parenthesis is missing and the compilation stops. RStudio gives us a hint about the location of the error (we can click on 'output' to have more details).

• Let's fix the parenthesis:

 Again, the compilation stops. We can have information about the error as previously for the missing parenthesis.

• Let's fix the column name:

• Again, the compilation stops. cor.test runs fine but inserts a tab character in the output that bothers LaTeX.

• It means we have to manually get the results:

#### **Tables**

 Tables can easily be printed using the xtable package (installed by typing install.packages("xtable")):

```
\section{Comparison of the studies}

<<label=comparison>>=
library(xtable)
theirs = c("Smurfs", "unknown proxy", "potential conflict of
interest")
ours = c("Moomins", "paintball activity", "no conflict of
interest")
comparison = data.frame(Haribo.et.al = theirs, our.study = ours)
print(xtable(comparison, caption = "Comparison of the studies"))
@
```

- Reference code for the rest of this practical is available in the file moomin\_reference\_advanced.Rnw
- A table of contents can be automatically inserted with the \tableofcontents command:

\maketitle

\tableofcontents

\section{Context of the study}

 Idem for the lists of figures and tables with the \listoffigures and \listoftables commands:

```
\maketitle
\tableofcontents
\listoffigures
\listoftables
\section{Context of the study}
```

• The list of figures is empty, we will see why and fix it later.

 We can add hyperlinks within the document with the hyperref LaTeX package:

```
\documentclass{article}
\usepackage[pdfborder={0 0 0}]{hyperref}
\title{Effect of lakritsi on agressiveness: a Moomin perspective}
```

We can the document margins with the geometry LaTeX package:

```
\usepackage[margin=3.5cm]{geometry}
```

 For LaTeX to be aware of the figures, we must insert them in a figure environment:

```
\begin{figure}
\begin{center}
<<label=plotSniffActivity, fig=TRUE, echo=FALSE>>=
Extract Sniff activity
sniff_activity = subset(paintball, paintball$user == "Sniff")
plot(sniff_activity$time.min, sniff_activity$balls.used, type =
"1")
@
\end{center}
\caption{Example of individual activity: Sniff}
\label{fig.Sniff.activity}
\end{figure}
```

• The label from the figure environment enables to refer to it from another part of the text:

The plot in Figure \ref{fig.Sniff.activity} shows the amount of balls used by Sniff during the game.

 LaTeX takes care of placing the figures and updating the references and links. However, this means the figure can be placed before or after the text referring to it.

LaTeX can also handle bibliography:

```
Haribo et al. \cite{haribo_liquorice_1973} have suggested a correlation between the consumption of \textbf{liquorice} and \textbf{agressive behaviour}, but their previous study on Smurfs (\textit{Schtroumpfus peyoii}) remained inconclusive.
```

At the end of the file:

```
\bibliographystyle{unsrt}
\bibliography{myLibrary}
\end{document}
```

• LaTeX will load the bibliography from myLibrary.bib.

#### **Summary**

- LaTeX is powerful but harder to learn than markdown.
- The plain-text files tend to be less human readable.
- LaTeX provides tools for more elaborated documents with table of contents and lists of figures, hyperlinks, automatic numbering and bibliography.

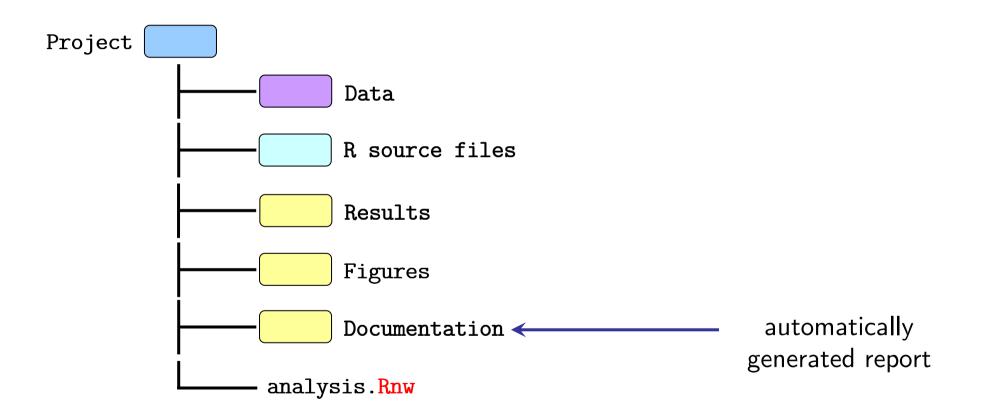
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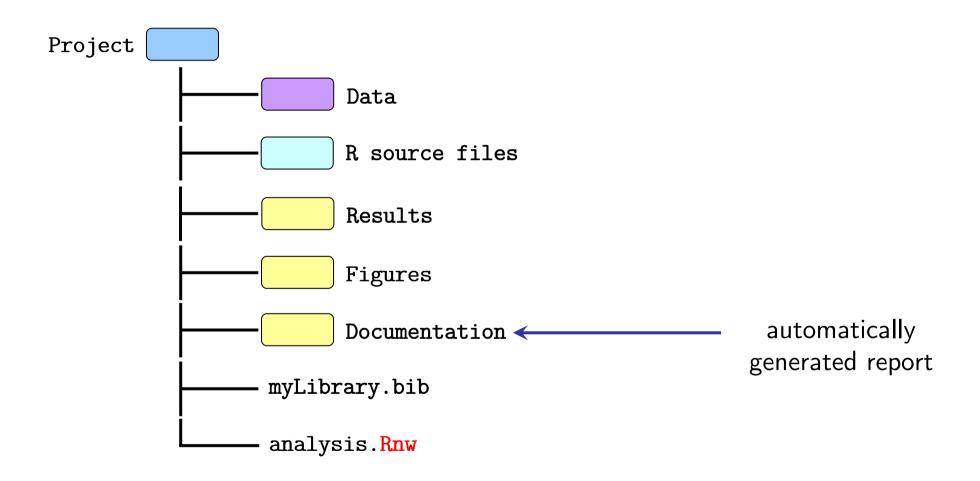
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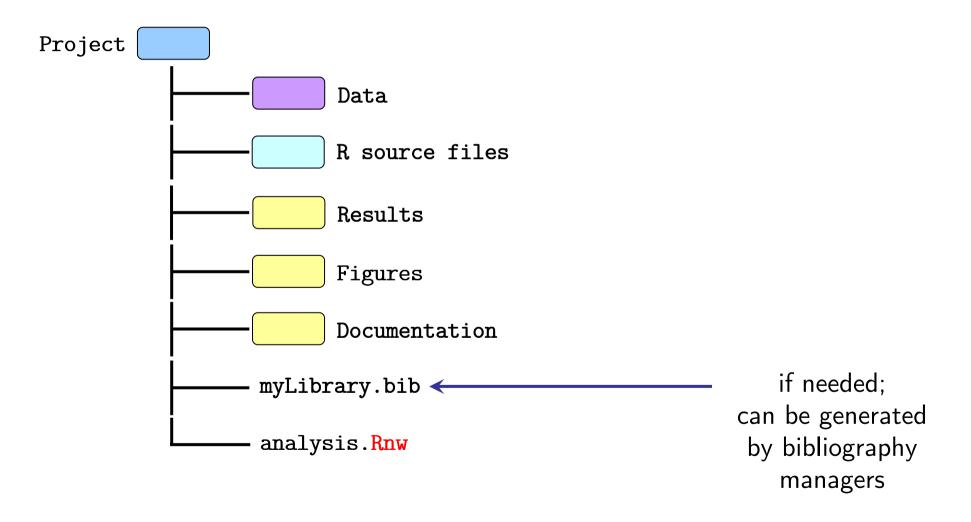
## **Examples of project folder**



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#### In brief

- Report generation guarantees that the results you are looking at have been generated by the exact code embedded in the same file.
- A report is updated by running the source file when data or analysis code change.
- Associating version control and report generation ensures having up-to-date documents, where everything is (in theory) traceable.

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## Further reading and references

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#### **RStudio documentation**

• Links for Sweave, knitr and R markdown documentation:

http://rstudio.com/ide/docs/

#### knitr

Project homepage with lots of resources:

http://yihui.name/knitr/

Tutorials can easily be found on the internet.

# Next Part Figure generation with make